

Quantum dark solitons in the 1D Bose gas and the superfluid velocity

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(Dated: March 2, 2013)

We give explicit connections of quantum one-hole excited states to classical solitons for the one-dimensional Bose gas with repulsive short-range interactions. We call the quantum states connected to classical solitons the *quantum soliton states*. We show that the matrix element of the canonical field operator between quantum soliton states with $N - 1$ and N particles is given by a dark soliton of the Gross-Pitaevskii equation in the weak coupling case. We suggest that the matrix element corresponds to the order parameter of BEC in the quantum soliton state. The result should be useful in the study of many-body effects in Bose-Einstein condensation and superfluids. For instance, we derive the superfluid velocity for a quantum soliton state.

PACS numbers: 03.75.Kk, 03.75.Lm

The experimental realization of trapped one-dimensional atomic gases has provided a new motivation in the study of the effects of strong correlations in fundamental quantum mechanical systems of interacting particles [1–3]. Furthermore, localized excitations in quantum many-body systems such as in cold atoms and optical lattices have recently attracted much interest and have been studied extensively in terms of “quantum solitons” [4, 5]. Localized quantum states are important and useful for investigating quite complicated excited states of interacting quantum systems. However, it is not clear how we can construct or characterize quantum states associated with solitons for many-body systems. Originally, solitons are special solutions of some classical nonlinear partial-differential equations. It is not even trivial to see whether there exists a quantum state with a soliton-like density profile.

Let us consider the Gross-Pitaevskii (GP) equation which describes Bose-Einstein condensation (BEC) in the mean-field approximation [6]. We also call it the classical nonlinear Schrödinger equation, since it corresponds to the classical limit of the quantum nonlinear Schrödinger equation satisfied by the canonical Bose field $\hat{\psi}(x, t)$ for the one-dimensional Bose gas interacting with the delta-function potentials. Here, the system is called the Lieb-Liniger (LL) model [7]. The GP equation has dark soliton solutions for the repulsive interactions, while it has bright soliton solutions for the attractive interactions [8]. It was conjectured that dark solitons are identified with Lieb’s type-II excitations as an excitation branch [9]. However, it has not been shown how one can construct such quantum states that are related to solitons or what kind of physical quantity can show a property of solitons for some states. In fact, each of the type-II eigenstates has a flat density profile, since the Bethe eigenstates are translationally invariant. Here we remark that for the attractive case, bright solitons are analytically derived from some quantum states of the LL model [10].

In this Letter we demonstrate that quantum states which are tightly connected to classical solitons are constructed from the Bethe eigenvectors of the LL model. We call the states the *quantum soliton states*. Let us denote by $\psi_{\text{QS}}(x)$ the matrix element of the field operator $\hat{\psi}(x, t)$ between two quantum soliton states where one state has $N - 1$ particles and another N particles. We show that the matrix element $\psi_{\text{QS}}(x)$ is well approximated by the classical complex scalar field of a dark soliton of the GP equation in the weak coupling case. We suggest that the matrix element $\psi_{\text{QS}}(x)$ corresponds to the order parameter of BEC in the system with a large but finite number of interacting particles in the weak coupling case. The result should be fundamental in the study of many-body effects in BEC and superfluids. For an illustration, we derive the superfluid velocity from the phase profile of the matrix element $\psi_{\text{QS}}(x)$.

We give remarks. First, superposing Lieb’s type II excitations, i.e. one-hole excitations, we construct the quantum soliton states [11], which have broken translational symmetry. The Bethe eigenstates are translationally invariant, while their superpositions are not, in general. Secondly, we show that the amplitude and phase profiles of quantum soliton states are consistent with those of corresponding solitons of the GP equation. Although the density profile with a density notch has been derived for a quantum soliton state [11], the connection to solitons has not been shown, yet. Thirdly, it is not *a priori* clear how valid the mean-field approximation is for the quantum soliton states. The exact wavefunctions given by the Bethe ansatz consist of a large number of terms such as $N!$. However, evaluating the matrix element $\psi_{\text{QS}}(x)$ we identify it as the order parameter of BEC.

Let us consider the Hamiltonian of the LL model [7]:

$$\mathcal{H}_{\text{LL}} = - \sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{j < k}^N \delta(x_j - x_k). \quad (1)$$

Here the periodic boundary conditions (P.B.C.) of the system size L are assumed on the wavefunctions. Hereafter, we consider the repulsive interaction: $c > 0$. The LL model is characterized by a single parameter $\gamma := c/n$, where $n = N/L$ is the particle density. We employ a system of units with $2m = \hbar = 1$, where m is the particle mass. The second-quantized Hamiltonian of the LL model is written in terms of the canonical Bose field $\hat{\psi}(x, t)$ as

$$\mathcal{H}_{\text{NLS}} = \int_0^L dx [\partial_x \hat{\psi}^\dagger \partial_x \hat{\psi} + c \hat{\psi}^\dagger \hat{\psi}^\dagger \hat{\psi} \hat{\psi} - \mu \hat{\psi}^\dagger \hat{\psi}], \quad (2)$$

where μ is the chemical potential. The Heisenberg equation of motion is called the nonlinear Schrödinger equation: $i\partial_t \hat{\psi} = -\partial_x^2 \hat{\psi} + 2c \hat{\psi}^\dagger \hat{\psi} \hat{\psi} - \mu \hat{\psi}$.

In the LL model, the Bethe ansatz offers an exact eigenstate with an exact energy eigenvalue for a given set of quasi-momenta k_1, k_2, \dots, k_N satisfying the Bethe equations for $j = 1, 2, \dots, N$:

$$k_j L = 2\pi I_j - 2 \sum_{\ell \neq j}^N \arctan \left(\frac{k_j - k_\ell}{c} \right). \quad (3)$$

Here I_j 's are integers for odd N and half-odd integers for even N . We call them the Bethe quantum numbers. The total momentum P and energy eigenvalue E are written in terms of the quasi-momenta as $P = \sum_{j=1}^N k_j = \frac{2\pi}{L} \sum_{j=1}^N I_j$, $E = \sum_{j=1}^N k_j^2$. If we specify a set of Bethe quantum numbers $I_1 < \dots < I_N$, the Bethe equations (3) have a unique real solution $k_1 < \dots < k_N$ [12].

Let us formulate quantum soliton states [11]. We shall show throughout the Letter that they lead to dark solitons of the GP equation. In the type II branch, for each integer p in the set $\{0, 1, \dots, N-1\}$, we consider momentum $P = 2\pi p/L$ and denote by $|P, N\rangle$ the normalized Bethe eigenstate of N particles with total momentum P . The Bethe quantum numbers of $|P, N\rangle$ are given by $I_j = -(N+1)/2 + j$ for integers j with $1 \leq j \leq N-p$ and $I_j = -(N+1)/2 + j + 1$ for j with $N-p+1 \leq j \leq N$. For each integer q satisfying $0 \leq q \leq N-1$ we define the coordinate state $|X, N\rangle$ of $X = qL/N$ by the discrete Fourier transformation:

$$|X, N\rangle := \frac{1}{\sqrt{N}} \sum_{p=0}^{N-1} \exp(-2\pi i p q / N) |P, N\rangle. \quad (4)$$

The density profile of the quantum soliton state, $\langle X, N | \hat{\psi}^\dagger(x) \hat{\psi}(x) | X, N \rangle$ versus x , is plotted in Fig. 1. It is denoted by ‘‘Many-body’’. Here we have set the coordinate integer as $q = 0$, and the density notch is localized at $x = L/2$. The expectation values of the density operator are effectively calculated [11] by the determinant formula for the norms of Bethe eigenstates [13] and that of the form factors of the density operator [14, 15].

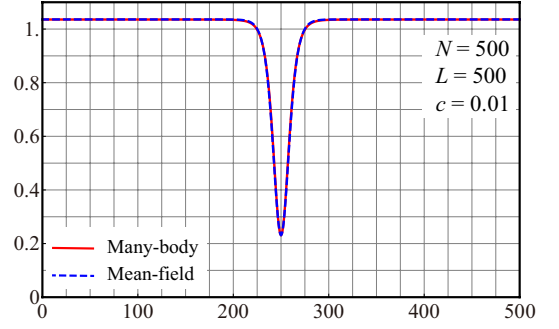


FIG. 1: (Color online) Density profile of the quantum soliton state $\langle X, N | \hat{\psi}^\dagger(x) \hat{\psi}(x) | X, N \rangle$ for $c = 0.01$ and $N = L = 500$ is shown by a red solid line. The profile of the squared amplitude of a dark soliton $|\psi_{\text{MF}}(x)|^2$ with $v \simeq v_c/2$ is plotted with a blue broken line.

The classical complex scalar field of a dark soliton solution for the GP equation with P.B.C., $\psi_{\text{MF}}(x)$ ($0 \leq x \leq L$), is derived by assuming the traveling-wave solution: $\psi(x, t) = \psi_{\text{MF}}(x - vt)$. Here we note that the periodic soliton solutions of the GP equation are expressed in terms of the elliptic integrals [5]. We also note that the excitation mode has the largest velocity v_c , which we call the critical velocity: there is no soliton solution with $v > v_c$ [5, 8, 9]. In the LL model, the critical momentum $p_c = mv_c$ corresponds to the Fermi momentum $2k_F$.

The density profile of the quantum soliton state and the square-amplitude profile of a classical dark soliton with P.B.C., $|\psi_{\text{MF}}(x)|^2$, agree quite well in the weak coupling case $c \ll 1$, as shown in Fig. 1. Here we have set $v \simeq v_c/2$ for the dark soliton, and its profile is denoted by ‘‘Mean-field’’.

We suggest that the soliton velocity $v \simeq v_c/2$ is consistent with the construction (4) of the quantum soliton state. Each of the type II excitations in the range $0 \leq v \leq v_c$ is superposed with equal weight, so that we have the average value $v \simeq v_c/2$. It looks like a wave packet of the type II excitations.

Let us consider the matrix element of the field operator between the quantum soliton states

$$\begin{aligned} \psi_{\text{QS}}(x) &:= \langle X, N-1 | \hat{\psi}(x) | X, N \rangle \\ &= \frac{1}{\sqrt{N(N-1)}} \sum_{p=0}^{N-1} \sum_{p'=0}^{N-2} e^{i(P-P')x} \langle P', N-1 | \hat{\psi}(0) | P, N \rangle, \end{aligned} \quad (5)$$

where $P = 2\pi p/L$ and $P' = 2\pi p'/L$ denote the total momenta of the normalized Bethe eigenstates $|P, N\rangle$ and $|P', N\rangle$, respectively. We put $q = 0$ in eq. (5). The matrix element $\langle P', N-1 | \hat{\psi}(0) | P, N \rangle$ are evaluated effectively by the determinant formula for the norms of Bethe eigenstates [13] and that for the form factors of

the field operator [15–17] as

$$\begin{aligned} \langle P', N-1 | \hat{\psi}(0) | P, N \rangle &= (-1)^{N(N+1)/2+1} \\ &\times \left(\prod_{j=1}^{N-1} \prod_{\ell=1}^N \frac{1}{k'_j - k_\ell} \right) \left(\prod_{j>\ell}^N k_{j,\ell} \sqrt{k_{j,\ell}^2 + c^2} \right) \\ &\times \left(\prod_{j>\ell}^{N-1} \frac{k'_{j,\ell}}{\sqrt{(k'_{j,\ell})^2 + c^2}} \right) \frac{\det U(k, k')}{\sqrt{\det G(k) \det G(k')}}, \quad (6) \end{aligned}$$

where the quasi-momenta $\{k_1, \dots, k_N\}$ and $\{k'_1, \dots, k'_{N-1}\}$ give the eigenstates $|P, N\rangle$ and $|P', N-1\rangle$, respectively. Here we have employed the abbreviated symbols $k_{j,\ell} := k_j - k_\ell$ and $k'_{j,\ell} := k'_j - k'_\ell$. The matrix $G(k)$ is the Gaudin matrix, whose (j, ℓ) th element is $G(k)_{j,\ell} = \delta_{j,\ell} \left[L + \sum_{m=1}^N K(k_{j,m}) \right] - K(k_{j,\ell})$ for $j, \ell = 1, 2, \dots, N$, where the kernel $K(k)$ is defined by $K(k) = 2c/(k^2 + c^2)$. The matrix elements of the $(N-1)$ by $(N-1)$ matrix $U(k, k')$ are given by

$$\begin{aligned} U(k, k')_{j,\ell} &= 2\delta_{j,\ell} \text{Im} \left[\frac{\prod_{a=1}^{N-1} (k'_a - k_j + ic)}{\prod_{a=1}^N (k_a - k_j + ic)} \right] \\ &+ \frac{\prod_{a=1}^{N-1} (k'_a - k_j)}{\prod_{a \neq j}^N (k_a - k_j)} (K(k_{j,\ell}) - K(k_{N,\ell})). \quad (7) \end{aligned}$$

The profiles of the squared amplitude $|\psi_{\text{QS}}(x)|^2$ and the phase $\text{Arg}[\psi_{\text{QS}}(x)]/\pi$ are plotted in Figs. 2 and 3 for $N = 20$ and 500, respectively. The squared amplitude and phase profiles of periodic dark solitons, $\psi_{\text{MF}}(x)$, are shown by broken blue lines in Figs. 2 and 3 for $N = 20$ and 500, respectively. They have the velocity $v \simeq 2\pi/L$. Here the classical complex scalar field $\psi_{\text{MF}}(x)$ is normalized such that the integral of $|\psi_{\text{MF}}(x)|^2$ with x over the whole region gives the particle number N .

The matrix element of the field operator, $\psi_{\text{QS}}(x)$, and the classical dark soliton with P.B.C., $\psi_{\text{MF}}(x)$, are in good agreement around the central part of the solitons in Figs. 2 and 3. In particular, the phase profiles of $\psi_{\text{QS}}(x)$ and $\psi_{\text{MF}}(x)$ completely overlap each other (see, the lower panels of Figs. 2 and 3). The profiles of square-amplitude $|\psi_{\text{QS}}(x)|^2$ of the quantum soliton states are slightly smaller than those of the periodic solitons, $|\psi_{\text{MF}}(x)|^2$, (see, the upper panels of Figs. 2 and 3). For $N = 20$ and $c = 0.01$ the two profiles are proportional to each other only with different normalizations. For $N = 500$ and $c = 0.01$ the two profiles overlap each other at the central part and deviate around at the shoulders.

The agreement of the squared amplitudes $|\psi_{\text{QS}}(x)|^2$ and $|\psi_{\text{MF}}(x)|^2$ should be improved for smaller values of c . Let us consider the form-factor expansion of the local density at x for the state $|X, N\rangle$:

$$\begin{aligned} \langle X, N | \hat{\psi}^\dagger(x) \hat{\psi}(x) | X, N \rangle \\ = |\psi_{\text{QS}}(x)|^2 + \sum_{|n\rangle \neq |X, N-1\rangle} |\langle n | \hat{\psi}(x) | X, N \rangle|^2. \quad (8) \end{aligned}$$

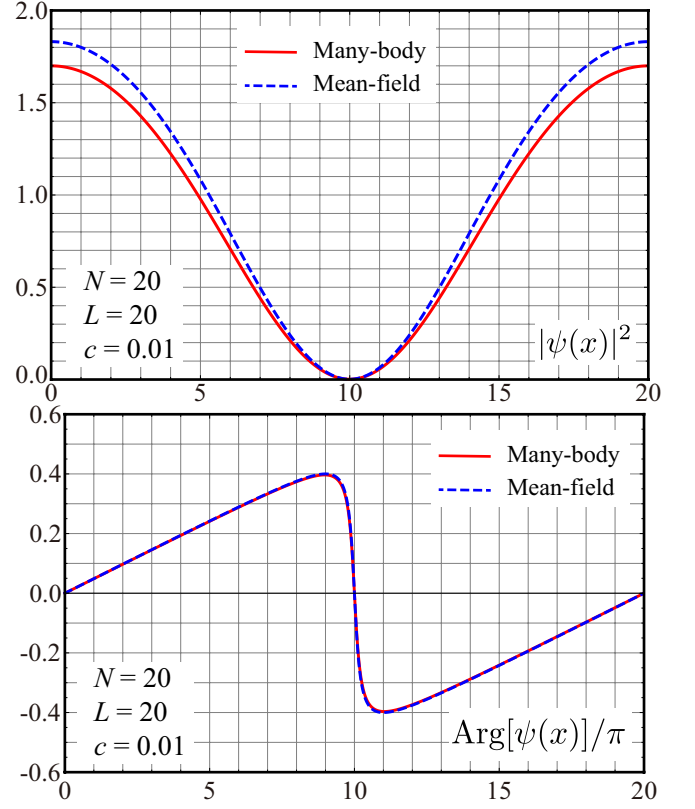


FIG. 2: (Color online) Profiles of the squared amplitude $|\psi_{\text{QS}}(x)|^2$ and the phase $\text{Arg}[\psi_{\text{QS}}(x)]/\pi$ for the matrix element of the field operator, $\psi_{\text{QS}}(x)$, are shown by red solid lines for $c = 0.01$ and $N = L = 20$. Those of a dark soliton under P.B.C., $\psi_{\text{MF}}(x)$, with $v \simeq 2\pi/L$ are plotted with blue dotted lines. Here we put $q = 0$.

The second terms of the right hand side of (8) give corrections to $|\psi_{\text{QS}}(x)|^2$, and the integral of $|\psi_{\text{QS}}(x)|^2$ with x over the whole region is smaller than the particle number N . We observed numerically that the correction terms become small as the coupling constant c decreases if we fix the particle number N , while they increase as N increases if c is fixed. In the large N case, the correction terms should be small if the value of c is small enough. We thus conclude that the matrix element $\psi_{\text{QS}}(x)$ is well approximated by the periodic dark soliton $\psi_{\text{MF}}(x)$ in the weak coupling case.

We suggest that the soliton velocity $v \simeq 2\pi/L$ corresponds to the difference between the average values of the total momenta of the quantum soliton states $|X, N\rangle$ and $|X, N-1\rangle$. It is consistent with the structure of the matrix element $\langle X, N-1 | \hat{\psi}(x) | X, N \rangle$.

We now argue for the claim that the matrix element $\psi_{\text{QS}}(x)$ gives the order parameter of BEC in the quantum soliton state $|X, N\rangle$ for the weak coupling and large- N case. Here the system size L is also very large since we set $n = N/L = 1$. We denote by $\rho_1(x, y)_{|\Psi\rangle}$ the one-particle reduced density matrix for a given state

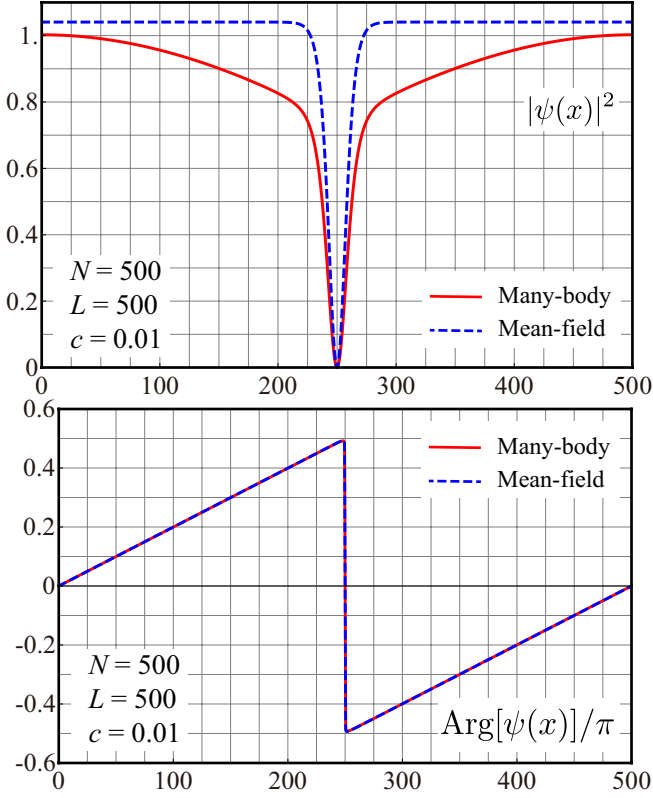


FIG. 3: (Color online) Same plots as in Fig. 2 with the system size $N = L = 500$.

$|\Psi\rangle$: $\rho_1(x, y)_{|\Psi\rangle} = \langle \Psi | \hat{\psi}^\dagger(x) \hat{\psi}(y) | \Psi \rangle$. We now conjecture that the matrix element $\psi_{\text{QS}}(x)$ satisfies the relation: $\rho_1(x, y)_{|X, N\rangle} \simeq \psi_{\text{QS}}^*(x) \psi_{\text{QS}}(y)$ for $|x - y| \gg 1$. We call it conjecture A. Here we assume that the system size L is much larger than the healing length $\ell_c = 1/\sqrt{cn}$. For instance, $\ell_c = 10$ for $c = 0.01$ and $n = 1$.

Suppose that the one-particle reduced density matrix $\rho_1(x, y)_{|\Psi\rangle}$ for a given state $|\Psi\rangle$ is diagonalized as

$$\rho_1(x, y)_{|\Psi\rangle} = \sum_i n_i \chi_i^*(x) \chi_i(y). \quad (9)$$

For the ground state we can numerically show that for small c the largest eigenvalue n_0 of $\rho_1(x, y)$ is much larger than the other eigenvalues: $n_0 \gg n_i$ for $i \neq 0$, i.e. the existence of BEC [11]. For the state $|X, N\rangle$ it could be technically nontrivial to diagonalize $\rho_1(x, y)_{|X, N\rangle}$ numerically. However, instead of doing it we point out that conjecture A is consistent with the following observation: The quantum soliton state $|X, N - 1\rangle$ is dominant among the intermediate states in the expansion (8). Here, we estimate the fraction of the correction term from the difference between the local density at x for the state $|X, N\rangle$ and the squared amplitude $|\psi_{\text{QS}}(x)|^2$, and it is small for small c and large N . Moreover, from the difference we estimate the condensate depletion, i.e. the fraction of the non-condensate components. It should have the largest

values for $x = y$, since the local density at x gives the diagonal element of $\rho_1(x, y)_{|X, N\rangle}$ with $x = y$.

We therefore conjecture that for small c and large N the order parameter $\sqrt{n_0} \chi_0(x)$ of the quantum soliton state $|X, N\rangle$ is given by the matrix element $\psi_{\text{QS}}(x)$, which is well approximated by the periodic dark soliton $\psi_{\text{MF}}(x)$ with $v \simeq 2\pi/L$. Here, the order parameter $\sqrt{n_0} \chi_0(x)$ has been defined by eq. (9) for $|\Psi\rangle = |X, N\rangle$. In terms of BEC we have connected the dark soliton $\psi_{\text{MF}}(x)$ with $v \simeq 2\pi/L$ to the state $|X, N\rangle$. It was not trivial to specify the soliton velocity v .

Let us now derive the superfluid velocity for a quantum soliton state $|X, N\rangle$. For large N such as $N = 500$, the phase field is fitted by $\theta(x) = \pi x/L - \pi H(x - X - L/2)$, as shown in the lower panel of Fig. 3. Here $H(x)$ denotes Heaviside's step function: $H(x) = 1$ for $x \geq 0$, and $H(x) = 0$ otherwise. Numerically we observed that the phase profile does not depend on the value of c for large N and small c . We derive the superfluid velocity from the phase field of the macroscopic wavefunction, $\theta(x)$, by $v_s = 2(\hbar/2m)(d\theta/dx)$ [18]. For large N we thus have

$$v_s = \frac{2\pi}{L} - \pi \delta(x - X - L/2). \quad (10)$$

The superfluid velocity v_s has a singularity at the location of the soliton, and is consistent with the soliton velocity $v \simeq 2\pi/L$.

The finding in the Letter suggests several possible future researches in quantum dynamics such as the collision of two quantum solitons, which is nontrivial in the dynamics of interacting quantum systems [19].

In conclusion, in order to prove that the quantum states $|X, N\rangle$ constructed in (4) for the 1D Bose gas are closely connected to classical solitons, we have shown the following two points: First, the density profile of the state $|X, N\rangle$ is consistent with the profile of the squared amplitude $|\psi_{\text{MF}}(x)|^2$ of the periodic dark soliton of the GP equation with $v \simeq v_c/2$. Then, the matrix element of the Bose field operator, $\psi_{\text{QS}}(x) = \langle X, N - 1 | \hat{\psi}(x) | X, N \rangle$, coincides with the classical complex scalar field $\psi_{\text{MF}}(x)$ of the dark soliton of the GP equation under P.B.C. with $v \simeq 2\pi/L$. The agreement is good for small c . Furthermore, we suggest that the matrix element $\psi_{\text{QS}}(x)$ gives the order parameter of BEC in the quantum soliton state $|X, N\rangle$ for small c and large N .

The authors thank I. Danshita and K. Sakai for their useful discussions. J.S. and E.K. are supported by JSPS.

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- [1] A. Görlitz, J.M. Vogels, A.E. Leanhardt, C. Raman, T.L. Gustavson, J.R. Abo-Shaeer, A.P. Chikkatur, S. Gupta, S. Inouye, T. Rosenband and W. Ketterle, Phys. Rev. Lett. **87**, 130402 (2001).
 - [2] M. Greiner, I. Bloch, O. Mandel, T.W. Hänsch, and T. Esslinger, Phys. Rev. Lett. **87**, 160405 (2001).

- [3] T. Kinoshita, T. Wenger and D.S. Weiss, *Science* **305**, 1125 (2004); *Phys. Rev. Lett.* **95**, 190406 (2005); *Nature* **440**, 900 (2006).
- [4] R.V. Mishmash and L.D. Carr, *Phys. Rev. Lett.* **103**, 140403 (2009); R.V. Mishmash, I. Danshita, C.W. Clark and L.D. Carr, *Phys. Rev. A* **80**, 053612 (2009).
- [5] R. Kanamoto, L.D. Carr, M. Ueda, *Phys. Rev. A* **79**, 063616 (2009); **81**, 023625 (2010).
- [6] A.J. Leggett, *Rev. Mod. Phys.* **73** (2001) 307–356.
- [7] E. H. Lieb and W. Liniger, *Phys. Rev.* **130**, 1605 (1963); E. H. Lieb, *Phys. Rev.* **130**, 1616 (1963).
- [8] T. Tsuzuki, *J. Low Temp. Phys.* **4**, 441 (1971); V.E. Zakharov, A.B. Shabat, *Sov. Phys.-JETP* **34**, 62 (1972).
- [9] M. Ishikawa and H. Takayama, *J. Phys. Soc. Jpn.* **49**, 1242 (1980).
- [10] C.R. Nohl, *Ann. Phys.* **96**, 234 (1976); M. Wadati, M. Sakagami, *J. Phys. Soc. Jpn.* **53**, 1933 (1984); M. Wadati, A. Kuniba, T. Konishi, *J. Phys. Soc. Jpn.* **54**, 1710 (1985); M. Wadati, A. Kuniba, *J. Phys. Soc. Jpn.* **55**, 76 (1986).
- [11] J. Sato, R. Kanamoto, E. Kaminishi, and T. Deguchi, *Phys. Rev. Lett.* **108**, 110401 (2012).
- [12] V.E. Korepin, N.M. Bogoliubov and A.G. Izergin, *Quantum Inverse Scattering Method and Correlation Functions* (Cambridge University Press, Cambridge, 1993)
- [13] M. Gaudin, “La fonction d’onde de Bethe”, Masson (Paris) (1983); V. E. Korepin, *Commun. Math. Phys.* **86**, 391 (1982).
- [14] P. Calabrese and J.-S. Caux, *J. Stat. Mech.* (2007) P08032.
- [15] N. A. Slavnov, *Teor. Mat. Fiz.* **79**, 232 (1989); **82**, 389 (1990).
- [16] J.-S. Caux, P. Calabrese and N. A. Slavnov, *J. Stat. Mech.* P01008 (2007).
- [17] T. Kojima, V.E. Korepin, N.A. Slavnov, *Commun. Math. Phys.* **188**, 657 (1997).
- [18] A.J. Leggett, *Quantum Liquids* (Oxford Univ. Press, 2006).
- [19] Q.Y. He, M.D. Reid, B. Opanchuk, R. Polkinghorne, Laura E. C. Rosales-Zarate, P.D. Drummond, arXiv:1112.0380 .